Growth modeling of InAs: Homoepitaxy and Sb adsorption

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Interface formation is critical for the quality of devices based on the 6.1 Å class of materials. The possible formation of two different interface types and reconstruction related roughness are active areas of research.

We present the results of kinetic Monte Carlo (KMC) simulation based on *ab initio* density functional theory (DFT) in comparison to scanning tunneling microscopy for annealed surfaces and growth kinetics of InAs(001). Our general method for using DFT calculations as input for microscopic models describing thermodynamic equilibrium and growth kinetics on III/V semiconductor surfaces is explained. Simulated island nucleation on InAs in the low coverage regime is in excellent agreement with experiment (see Fig. 1). Furthermore, relevant microscopic processes for decrease of island number density and decrease of anisotropy with increasing As pressure are revealed: Suppression of effective In adatom density through incoming As leads to reduced island nucleation.

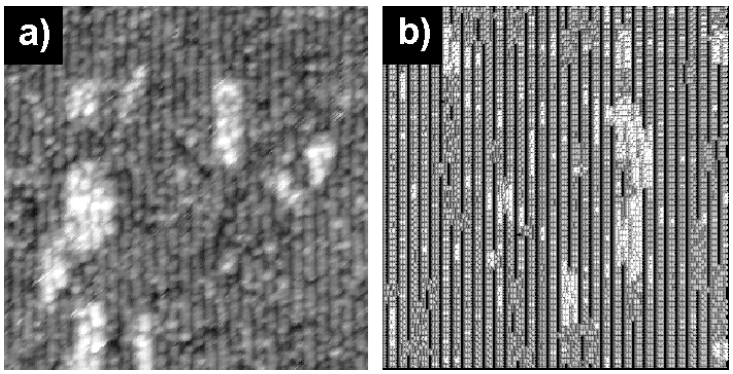

Fig 1: a) Filled-states constant current STM image (2 V bias, 0.1 nA) of an InAs(001) surface after 2 s growth at 380 C, F(As)=2.5 Ml/s, F(In)=0.073 ML/s, size: 55 nm x 55 nm. b) Surface morphology in KMC under identical conditions and identical size.

To investigate interface formation we study Sb adsorption on InAs(001). The reconstruction phase diagram for mixed As/Sb fluxes reveals a large number of stable reconstructions. Based on these results the possibilities of influencing the character of the interface bonds between InAs and AlSb/GaSb are discussed.

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[1] Bockstedte, Kley, Neugebauer, Scheffler, CPC **107**, 187 (1997). http://www.fhi-berlin.mpg.de/th/fhi98md/